

MxP® Quant 500 kit requirements

This document specifies additional lab equipment and chemicals that are required but not included with the kit. Before starting with the kit, ensure that all required items are available.

LC-MS system

Agilent	SCIEX	Waters
Mass spectrometer		
Agilent 6495B, 6495C Triple Quadrupole LC/MS System	SCIEX 5500, 5500+, 6500 or 6500+ series (QTRAP or Triple Quad) with TurboV™ ion source	Waters Xevo TQ-S or TQ-XS with ESI source
LC and autosampler		
<ul style="list-style-type: none"> – Agilent 1290 Infinity I/II UHPLC system with column oven. NanoLC and microLC are not supported! – 800 bar injection valve (Agilent part no. 5067-6698) replaces standard 1300 bar valve – 1290 Infinity II inline filters, 0.3 µm (2 pcs., before and after injection valve, Agilent part no. 5067-6189) – 96-well plate autosampler with temperature control (10 °C) – Injection volume range: 2 – 20 µL 	<ul style="list-style-type: none"> – Standard flow HPLC or UHPLC system with column oven. NanoLC and microLC are not supported! – 96-well plate autosampler with temperature control (10 °C) – Injection volume range: 5 – 20 µL – Special sample rack for deep-well plates required for the following autosamplers: <ul style="list-style-type: none"> – Shimadzu: part no. 228-37546-92 (Deep-well MTP Rack, DWP-96) – UltiMate 3000: Thermo part no. 6820.4083 (30 – 36 mm height) 	<ul style="list-style-type: none"> – Waters ACQUITY UPLC® system with sample manager, solvent manager, and column oven: <ul style="list-style-type: none"> – Classic (loop-based) – I-Class (FTN) – H-Class (FTN) – Injection volume range: 2 – 20 µL FTN samplers require extension loop of 50 µL or needle size of 30 µL!
Tubing		
<ul style="list-style-type: none"> – Recommended between injector and column system: steel capillary – Recommended between column system and mass spectrometer: red PEEK Tubing 1/16" OD x 0.005" ID 		

LC-MS instrument status

Condition
<ul style="list-style-type: none"> – Serviced, calibrated and tuned instruments according to manufacturer’s recommendations on a regular basis – LC-MS system must be free of ion-pair reagent

Analytical column

HPLC and UHPLC	
Analytical column	MxP® Quant 500 kit column system: biocrates product number 9120052121117 (HPLC/UHPLC column + pre-column mixer + connector, factory assembled)

Software

Agilent	SCIEX	Waters
MS software		
MassHunter version 10.1 or later	Analyst® version 1.5.2 or later	MassLynx® version 4.1 or later
Data processing computer		
<ul style="list-style-type: none"> – Oracle® database: <ul style="list-style-type: none"> – Option 1 (recommended): full commercial version, updates and support provided by Oracle. Expert required. Compatible versions: 11g, 12c, 18c, 21c. – Option 2: Oracle Database Express Edition (Oracle XE), free of charge, provided by biocrates. No updates and support provided by Oracle. Compatible versions: 11g, 12c, 18c, 21c – RAM for Oracle XE: Computer with up to 32 GB RAM. Contact biocrates support if a computer with more than 32 GB RAM is used. – MetIDQ™ software (provided by biocrates) – Windows 7 or later, 64-bit architecture – Microsoft .NET Framework 4.5.2 or later – Microsoft Visual C++ redistributables (32 & 64 bit each): 2005, 2008, 2010, 2012, and 2013 		

Solvents and chemicals

Solvents and chemicals	Purity
Ethanol, methanol, water, acetonitrile, isopropanol	LC-MS grade (ethanol: HPLC grade sufficient)
Formic acid	LC-MS grade (e.g. Honeywell Fluka™ 56302-50ML) Fresh! New bottle or opened within past 6 months
Phenyl isothiocyanate (PITC)	99%, for protein sequencing (e.g. Sigma-Aldrich 317861) Fresh! New bottle or opened within past 6 months
Pyridine	Purity >99% (recommended Acros Organics 131780500, 50mL) Fresh! New bottle or opened within past 6 months
Ammonium acetate	LC-MS grade
Phosphate buffered saline (PBS)	p.a. grade (e.g. Sigma-Aldrich P4417)

Laboratory equipment

Laboratory equipment		
	Nitrogen evaporator for 96-well plates	Pressure manifold for 96-well plates
Nitrogen evaporator* <u>or</u> pressure manifold* > Requires nitrogen supply > Must be in a fume hood	Examples: – Porvair blowdown evaporator MiniVap® – Techne (FSC496D) – Sample concentrator from BenchTop Lab Systems (96 samples, BT1604) – VLM evaporators – Organomation MICROVAP microplate evaporator – Biotage TurboVap® 96	Examples: – Waters positive pressure-96 processor (186006961) – Biotage® PRESSURE+ 96 manifold (PPM-96) – CEREX® system 96 processor (288-0001) – Agilent positive pressure manifold 96 processor (PPM-96) – TECAN Resolvex® M10 96
Centrifuge	Must be able to centrifuge 96-well plates of 5 cm height at 500 x g	Not required when a pressure manifold is used.
Shaker	Any model with adjustable speed (450 – 1200 rpm) including a tray for plates and vials. Recommended: Eppendorf MixMate® or ThermoMixer®	
Pipettes	– Repeater, e.g. Eppendorf Multipette® E3 (with 2.5 and 10 mL tips) or similar electronic model – Single channel: volume range 10 µL – 1000 µL – 8-Channel: 10 µL – 150 µL	
Vortexer	Any model	
Balance	Accuracy < 1 mg	
Solvent bottles	50 – 1000 mL	

* See document “Technical guide-Nitrogen evaporators and pressure manifolds” for details.